

Bounds for the Atom–Bond Sum–Connectivity Index of Graphs

Zaryab Hussain^a, Hechao Liu^{b,*}, Hongbo Hua^c

^a*School of Mathematics and Statistics, Northwestern Polytechnical
University, Xi'an, Shaanxi 710129, China*

^b*Huangshi Key Laboratory of Metaverse and Virtual Simulation, School
of Mathematics and Statistics, Hubei Normal University, Huangshi,
Hubei 435002, China*

^c*Faculty of Mathematics and Physics, Huaiyin Institute of Technology,
Huai'an, Jiangsu 223003, China*

zaryabhussain2139@gmail.com, hechaoliu@yeah.net, hongbo_hua@163.com

(Received March 28, 2024)

Abstract

The *atom-bond sum-connectivity* (*ABSC*) index of a graph G is defined as $ABSC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}}$, where d_u and d_v represent the degrees of u and v in G , respectively. In this paper, we give some sharp bounds for the *ABSC* index in terms of the first Zagreb index, the harmonic index, the sum-connectivity index, the minimum and maximum degrees, the clique number, and the chromatic number. We also find a lower bounds for the *ABSC* index of trees with given number of vertices and maximum degree.

1 Introduction

In chemical graph theory, vertices correspond to atoms, and edges correspond to bonds in a molecule. Using graphs, one can capture essential features of molecular structures and explore how they affect various chemical properties and behaviors [5, 8]. In graph-theoretical terms, a number

represents graph's structure is called a topological index. To measure the degree of branching of saturated hydrocarbons, in 1975 Randić introduced the Randić (R) index [28]. For a graph G the Randić index is defined as:

$$R(G) := \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}, \quad (1)$$

where d_u and d_v represent the degrees of u and v in G , respectively.

Estrada et al. [15] modified the Randić index by taking into consideration not only the degrees of the end-vertices of the edges, but also the degrees of the edges by introducing the atom-bond connectivity (ABC) index of graphs. This parameter was studied in the papers [1,6,9,12–14,17,19,22]. The ABC index of a graph G is defined as:

$$ABC(G) := \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \quad (2)$$

A probabilistic interpretation of the ABC index is given in [14]. It indicates that the terms defining this index represent the probability of visiting a nearest neighbor edge from one side or the other of a given edge in a graph.

On the other side, Zhou et al. [31] modified the Randić index by replacing $d_u d_v$ with $d_u + d_v$ in the formula (1), and named this new index the sum-connectivity index. For a graph G , the sum-connectivity (SC) index is defined as:

$$SC(G) := \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}. \quad (3)$$

By amalgamating the core idea of the atom-bond connectivity index and sum-connectivity index, Ali et al. [2,3] proposed the *atom-bond sum-connectivity* ($ABSC$) index of graphs. The $ABSC$ index of a graph G is defined as:

$$ABSC(G) := \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}}. \quad (4)$$

The formula (4) can also be written as:

$$ABSC(G) := \sum_{uv \in E(G)} \sqrt{1 - \frac{2}{d_u + d_v}}. \quad (5)$$

Several authors have been attracted towards the *ABSC* index in the last few years for example [4, 10, 11, 21, 23, 25–27, 30]. All these papers are related to extreme bounds for the *ABSC* index of graphs.

Let \mathcal{T}_n be the set of trees with n vertices and $\mathcal{T}_{n,\Delta}$ be the set of trees with n vertices and maximum degree Δ . Denote by P_n and S_n the path and star with n vertices, respectively. A *pendent vertex* in a graph is a vertex with degree one. A pendent vertex in a tree is also called a *leave*. A *stem* is a vertex adjacent to a pendent vertex. A *strong stem* is a stem adjacent to at least two pendent vertices. An *end-stem* is a stem whose all neighbors, except at most one, are pendent vertices. A vertex's *progenitor* (parent vertex) in a rooted tree is the vertex connected to it along the path to the root. The term *clique number* of a graph G refers to the number of vertices in a largest clique (the set of vertices with all pairs adjacent) and it is denoted as $\alpha(G)$. The *chromatic number* of a graph G is the least number of colors required to color all of its vertices while ensuring that no two neighboring vertices receive the same color. This number is represented by the symbol $\chi(G)$. For convenience, we will use $I(uv) = \sqrt{1 - \frac{2}{d_u + d_v}}$. Some significant results that will assist us in proving our primary findings are provided below.

Lemma 1. ([2]) *Let $n \geq 4$ and $T \in \mathcal{T}_n$. Then $ABSC(T) \geq ABSC(P_n)$, the equality holds if and only if $T \cong P_n$.*

A well-known inequality, the Diaz-Metcalf inequality, was first published in [24].

Lemma 2. ([24]) *Let a_i and b_i , where $i = 1, 2, \dots, n$, be real numbers such that $Aa_i \leq b_i \leq Ba_i$ for each $i = 1, 2, \dots, n$ with $0 < A \leq B$. Then*

$$(A + B) \sum_{i=1}^n a_i b_i \geq \sum_{i=1}^n b_i^2 + AB \sum_{i=1}^n a_i^2,$$

the equality holds if and only if either $b_i = Aa_i$ or $b_i = Ba_i$ for each $i = 1, 2, \dots, n$.

Lemma 3. ([20]) *Let a and b be real numbers such that $a \geq b \geq 0$. Then $\sqrt{a-b} \geq \sqrt{a} - \sqrt{b}$, the equality holds if and only if $a = b$ or $b = 0$.*

Lemma 4. ([29]) *Let G be a connected K_{q+1} -free graph of order n and having m edges. Then*

$$m \leq \left(1 - \frac{1}{q}\right) \cdot \frac{n^2}{2},$$

the equality holds if and only if G is a complete q -partite graph in which all classes are of equal cardinality.

For a graph G , the harmonic (H) index is defined as [16]:

$$H(G) := \sum_{uv \in E(G)} \frac{2}{d_u + d_v}. \quad (6)$$

Lemma 5. ([7]) *Let G be a simple graph with chromatic number $\chi(G)$ and harmonic index $H(G)$. Then $\chi(G) \leq 2H(G)$, the equality holds if and only if G is a complete graph possibly with some additional isolated vertices.*

The remainder of this paper is organized as follows: In Section 2, we obtain certain lower bounds for the *ABSC* index of graphs, specifically the least *ABSC* index of trees with a given maximum degree. In Section 3, we give some upper bounds for the *ABSC* index of graphs. In Section 4, we conclude our paper.

2 Lower bounds for the *ABSC* index of graphs

In this section, we will find lower bounds for the atom-bond sum-connectivity index of graphs.

Theorem 1. *Let G be a connected graph with m edges, maximum degree Δ and minimum degree δ . Then*

$$m\sqrt{\frac{\delta-1}{\Delta}} \leq ABSC(G) \leq m\sqrt{\frac{\Delta-1}{\delta}},$$

the equality holds if and only if G is a regular graph.

Proof. For $uv \in E(G)$, we have

$$\sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} = \sqrt{\frac{1}{d_u + d_v}} \cdot \sqrt{d_u + d_v - 2}.$$

It follows from

$$\sqrt{2(\delta-1)} \leq \sqrt{d_u + d_v - 2} \leq \sqrt{2(\Delta-1)}$$

and

$$\sqrt{\frac{1}{2\Delta}} \leq \sqrt{\frac{1}{d_u + d_v}} \leq \sqrt{\frac{1}{2\delta}}$$

Thus,

$$m\sqrt{\frac{\delta-1}{\Delta}} \leq ABSC(G) \leq m\sqrt{\frac{\Delta-1}{\delta}}.$$

Since $\delta = \Delta$ only holds when G is a regular graph and vice versa, the equalities only hold when G is a regular graph. ■

The first Zagreb (M_1) index [18] of a graph G is defined as:

$$M_1(G) := \sum_{uv \in E(G)} (d_u + d_v). \quad (7)$$

Theorem 2. *Let G be a connected graph with m edges, maximum degree Δ and minimum degree $\delta \geq 2$. Then*

$$ABSC(G) \geq \frac{M_1(G) + 2\sqrt{\delta\Delta(\delta-1)(\Delta-1)}H(G) - 2m}{2\left(\sqrt{\delta(\delta-1)} + \sqrt{\Delta(\Delta-1)}\right)}, \quad (8)$$

the equality holds if and only if G is a regular graph.

Proof. We know that

$$\sqrt{2(\delta-1)} \leq \sqrt{d_u + d_v - 2} \leq \sqrt{2(\Delta-1)},$$

$$\sqrt{\frac{1}{d_u + d_v}} \sqrt{2\delta} \sqrt{2(\delta-1)} \leq \sqrt{d_u + d_v - 2} \leq \sqrt{\frac{1}{d_u + d_v}} \sqrt{2\Delta} \sqrt{2(\Delta-1)},$$

and

$$\sqrt{\frac{1}{d_u + d_v}} 2\sqrt{\delta(\delta-1)} \leq \sqrt{d_u + d_v - 2} \leq \sqrt{\frac{1}{d_u + d_v}} 2\sqrt{\Delta(\Delta-1)}.$$

Setting $2\sqrt{\delta(\delta-1)}$ as A , $2\sqrt{\Delta(\Delta-1)}$ as B , $\sqrt{\frac{1}{d_u+d_v}}$ as a_i and $\sqrt{d_u + d_v - 2}$ as b_i , by Lemma 2 we have

$$\begin{aligned} ABSC(G) &= \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u + d_v}} \cdot \sqrt{d_u + d_v - 2} \\ &= \frac{[2\sqrt{\delta(\delta-1)} + 2\sqrt{\Delta(\Delta-1)}]}{2\sqrt{\delta(\delta-1)} + 2\sqrt{\Delta(\Delta-1)}} \sum_{uv \in E(G)} \left(\sqrt{\frac{1}{d_u + d_v}} \cdot \sqrt{d_u + d_v - 2} \right) \\ &\geq \frac{\left[\sum_{uv \in E(G)} (d_u + d_v - 2) + (4\sqrt{\delta(\delta-1)}\sqrt{\Delta(\Delta-1)}) \right] \left(\sum_{uv \in E(G)} \frac{1}{d_u + d_v} \right)}{2\sqrt{\delta(\delta-1)} + 2\sqrt{\Delta(\Delta-1)}} \\ &= \frac{M_1(G) + 2\sqrt{\delta\Delta(\delta-1)(\Delta-1)}H(G) - 2m}{2(\sqrt{\delta(\delta-1)} + \sqrt{\Delta(\Delta-1)})}. \end{aligned}$$

This completes the proof. ■

Theorem 3. Let G be a graph with n vertices and m edges. Then

$$ABSC(G) \geq m - \sqrt{2} SC(G), \quad (9)$$

the equality holds if and only if $G \cong \frac{n}{2}K_2$ (n is even).

Proof. By Lemma 3, we have

$$ABSC(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u + d_v}} \cdot \sqrt{d_u + d_v - 2}$$

$$\begin{aligned}
&\geq \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u + d_v}} \cdot (\sqrt{d_u + d_v} - \sqrt{2}) \\
&= \sum_{uv \in E(G)} - \sum_{uv \in E(G)} \sqrt{\frac{2}{d_u + d_v}} \\
&= m - \sqrt{2}SC(G),
\end{aligned}$$

where the equality holds if and only if $G \cong \frac{n}{2}K_2$ (n is even). This completes the proof. \blacksquare

Corollary. *Let G be a graph with n vertices, m edges and minimum degree δ . Then*

$$ABSC(G) \geq m \left(1 - \frac{1}{\sqrt{\delta}}\right),$$

the equality holds if and only if $G \cong \frac{n}{2}K_2$ (n is even).

Proof. Since

$$SC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \leq \frac{m}{\sqrt{2\delta}}, \quad (10)$$

from Theorem 3, we get the required result. Moreover the equality holds in (10) if and only if $G \cong \frac{n}{2}K_2$ (n is even). \blacksquare

Now we will find the minimum value of the $ABSC$ index of $T \in \mathcal{T}_{n,\Delta}$. We apply some transformations to streamline the problem of minimizing the $ABSC$ index of $T \in \mathcal{T}_{n,\Delta}$. From this point on, we assume that T is a rooted tree with root r and that r is a vertex with maximum degree Δ and $N(r) = \{r_1, r_2, \dots, r_\Delta\}$.

Theorem 4. *Let $n \geq 5$ and $T \in \mathcal{T}_{n,\Delta}$. Then we have*

$$\begin{aligned}
&ABSC(T) \geq \\
&\begin{cases} \Delta \left(\sqrt{\frac{\Delta}{\Delta+2}} + \sqrt{\frac{1}{3}} \right) + \frac{\sqrt{2}}{2} (n - 2\Delta - 1), & \Delta \leq \frac{n-1}{2}; \\ (n - \Delta - 1) \left(\sqrt{\frac{\Delta}{\Delta+1}} + \sqrt{\frac{1}{3}} \right) + (2\Delta - n + 1) \sqrt{\frac{\Delta-1}{\Delta+1}}, & \Delta > \frac{n-1}{2}. \end{cases}
\end{aligned}$$

Before we prove Theorem 4, we need to prove a few supporting results.

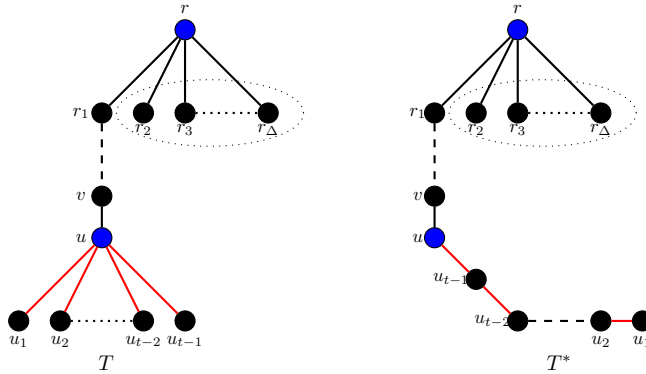


Figure 1. The trees T and T^* in the proof of Lemma 6.

Lemma 6. Let $T \in \mathcal{T}_{n,\Delta}$ be a rooted tree and r be the root vertex of T with $d_T(r) = \Delta$. If there is an end-stem with degree at least three other than the root vertex r in T , then there exists a tree T^* with $|V(T^*)| = n$ and $\Delta(T^*) = \Delta$, such that $ABSC(T) > ABSC(T^*)$.

Proof. Let $u \neq r$ be an end-stem of T with $d_T(u) = t \geq 3$. Suppose that v is the parent vertex of u and $N(u) = \{v, u_1, u_2, \dots, u_{t-1}\}$. Let $\Omega = \{uv, uu_1, uu_2, \dots, uu_{t-1}\}$ and $T^* = T - \{uu_1, uu_2, \dots, uu_{t-2}\} + \{u_1u_2, u_2u_3, \dots, u_{t-2}u_{t-1}\}$. Then $|V(T^*)| = n$ and $\Delta(T^*) = \Delta$, thus we have

$$\begin{aligned}
 ABSC(T) &= \sum_{uv \notin \Omega} I(uv) + \sum_{uv \in \Omega} I(uv) \\
 &= \sum_{uv \notin \Omega} I(uv) + \sqrt{1 - \frac{2}{t + d_T(v)}} + (t-2) \sqrt{1 - \frac{2}{t+1}} \\
 &\quad + \sqrt{1 - \frac{2}{t+1}}
 \end{aligned}$$

and

$$ABSC(T^*) = \sum_{uv \notin \Omega} I(uv) + \sqrt{1 - \frac{2}{2 + d_T(v)}} + (t-2) \sqrt{1 - \frac{2}{2+2}}$$

$$+ \sqrt{1 - \frac{2}{2+1}}.$$

Now using $d_T(u) = t \geq 3$, we get

$$\begin{aligned} ABSC(T) - ABSC(T^*) &\geq \sqrt{1 - \frac{2}{t + d_T(v)}} - \sqrt{1 - \frac{2}{2 + d_T(v)}} \\ &+ \sqrt{1 - \frac{2}{t + 1}} - \sqrt{1 - \frac{2}{2 + 1}} > 0. \end{aligned}$$

■

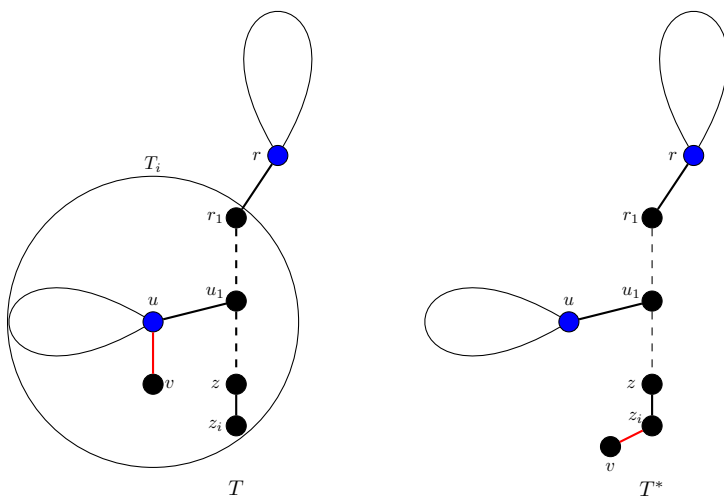


Figure 2. The trees T and T^* in the proof of Lemma 7.

Lemma 7. Let $T \in \mathcal{T}_{n,\Delta}$ be a rooted tree and r is the root vertex of T with $d_T(r) = \Delta$. If there is a stem with degree at least three other than the root vertex r in T , then there exists a tree T^* with $|V(T^*)| = n$ and $\Delta(T^*) = \Delta$, such that $ABSC(T) > ABSC(T^*)$.

Proof. Let $u \neq r$ be a stem of T with $d_T(u) = t \geq 3$ and $N(u) =$

$\{v, u_1, u_2, \dots, u_{t-1}\}$ where vertex u_1 is the parent of u and v is a pendent vertex in T . If u is an end-stem, then by Lemma 6, the conclusion holds. Thus we can assume that u is a stem, but not an end-stem. Let $rr_i \in E(T)$ and T_i be the component of $T - rr_i$ containing r_i . Let $z_i \in V(T_i)$ be one pendent vertex with maximum distance from r_i in T_i and vertex z is a parent of z_i . If $d_T(z) \geq 3$, then by Lemma 6, we can obtain a contradiction. Thus $d_T(z) = 2$. Let $\Omega = \{zz_i, uv, uu_1, uu_2, \dots, uu_{t-1}\}$ and $T^* = T - uv + vz_i$. Then $|V(T^*)| = n$ and $\Delta(T^*) = \Delta$, thus we have

$$\begin{aligned} ABSC(T) &= \sum_{uv \notin \Omega} I(uv) + \sum_{uv \in \Omega} I(uv) \\ &= \sum_{uv \notin \Omega} I(uv) + \sqrt{1 - \frac{2}{1+t}} + \sqrt{1 - \frac{2}{1+2}} \\ &\quad + \sum_{i=1}^{t-1} \sqrt{1 - \frac{2}{d_T(u_i) + t}} \end{aligned}$$

and

$$\begin{aligned} ABSC(T^*) &= \sum_{uv \notin \Omega} I(uv) + \sqrt{1 - \frac{2}{2+2}} + \sqrt{1 - \frac{2}{1+2}} \\ &\quad + \sum_{i=1}^{t-1} \sqrt{1 - \frac{2}{d_T(u_i) + t - 1}}. \end{aligned}$$

Now using $d_T(u) = t \geq 3$, we get

$$\begin{aligned} ABSC(T) - ABSC(T^*) &= \sqrt{1 - \frac{2}{1+t}} - \sqrt{1 - \frac{2}{2+2}} \\ &\quad + \sum_{i=1}^{t-1} \sqrt{1 - \frac{2}{d_T(u_i) + t}} \\ &\quad - \sum_{i=1}^{t-1} \sqrt{1 - \frac{2}{d_T(u_i) + t - 1}} > 0. \end{aligned}$$

■

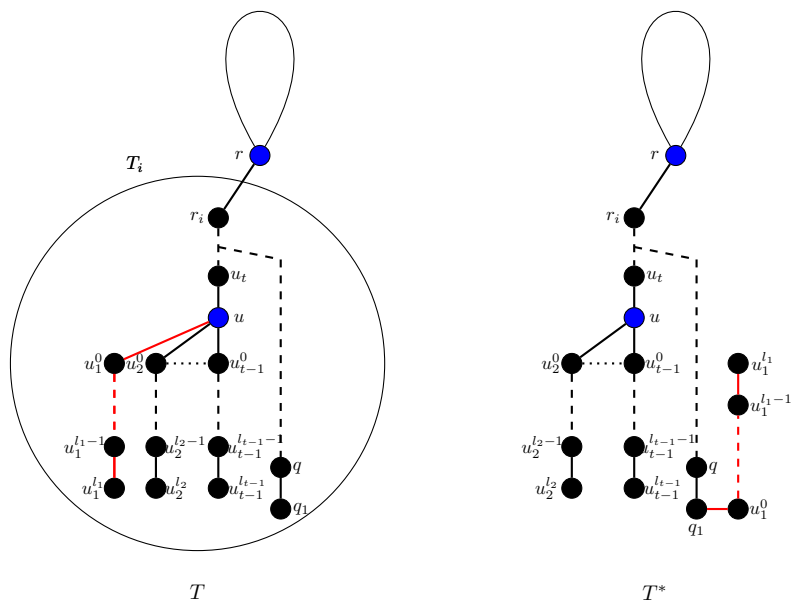


Figure 3. The trees T and T^* in the proof of Lemma 8.

Lemma 8. Let $T \in \mathcal{T}_{n,\Delta}$ be a rooted tree and r be the root vertex of T with $d_T(r) = \Delta$. If there is a vertex with degree at least three other than the root vertex r in T , then there exists a tree T^* with $|V(T^*)| = n$ and $\Delta(T^*) = \Delta$, such that $ABSC(T) > ABSC(T^*)$.

Proof. Let $u \neq r$ be a vertex with $d_T(u) = t \geq 3$ such that $d_T(u, r)$ is as large as possible. Assume $N(u) = \{u_1^0, u_2^0, \dots, u_{t-1}^0, u_t\}$, and u_t is the parent of vertex u . Let $rr_i \in E(T)$ and T_i be the component of $T - rr_i$ containing r_i . Suppose that the path $u_i^0 u_i^1 \dots u_i^{l_i}$ is the longest path in T_i starting from u_i^0 where $i = 1, 2, l, \dots, t-1$. Further suppose that $q_i \in V(T_i)$ is a pendent vertex such that $d_{T_i}(r_i, q_i)$ is maximum. Let q be the parent of vertex q_i . Now we can suppose that $q_i \notin \{u_1^{l_1}, \dots, u_{t-2}^{l_{t-2}}\}$. By Lemmas 6 and 7 and that $d_T(u, r)$ is as large as possible, $d_T(q) = 2$ and all descendants of u except pendent vertices, have degree two. We distinguish three cases:

Case 1. $t = 3$.

Let $T^* = T - uu_1^0 + q_i u_1^0$. Then we have $|V(T^*)| = n$ and $\Delta(T^*) = \Delta$.
Let $\Omega = \{q_i q, uu_1^0, uu_2^0, uu_3\}$. Then we have

$$\begin{aligned} ABSC(T) &= \sum_{uv \notin \Omega} I(uv) + \sum_{uv \in \Omega} I(uv) \\ &= \sum_{uv \notin \Omega} I(uv) + \sqrt{1 - \frac{2}{3+2}} + \sqrt{1 - \frac{2}{3+2}} \\ &\quad + \sqrt{1 - \frac{2}{3+d_T(u_3)}} + \sqrt{1 - \frac{2}{2+1}} \end{aligned}$$

and

$$\begin{aligned} ABSC(T^*) &= \sum_{uv \notin \Omega} I(uv) + \sqrt{1 - \frac{2}{2+2}} + \sqrt{1 - \frac{2}{2+2}} \\ &\quad + \sqrt{1 - \frac{2}{2+d_T(u_3)}} + \sqrt{1 - \frac{2}{2+2}}. \end{aligned}$$

Thus,

$$ABSC(T) - ABSC(T^*) > 2\sqrt{1 - \frac{2}{3+2}} + \sqrt{1 - \frac{2}{2+1}} - 3\sqrt{1 - \frac{2}{2+2}} > 0.$$

Case 2. $t = 4$.

Let $T^* = T - uu_1^0 + q_i u_1^0$. Then we have $|V(T^*)| = n$ and $\Delta(T^*) = \Delta$.
Let $\Omega = \{q_i q, uu_1^0, uu_2^0, uu_3^0, uu_4\}$. Then we have

$$\begin{aligned} ABSC(T) &= \sum_{uv \notin \Omega} I(uv) + \sum_{uv \in \Omega} I(uv) \\ &= \sum_{uv \notin \Omega} I(uv) + 3\sqrt{1 - \frac{2}{4+2}} + \sqrt{1 - \frac{2}{4+d_T(u_4)}} \\ &\quad + \sqrt{1 - \frac{2}{2+1}} \end{aligned}$$

and

$$ABSC(T^*) = \sum_{uv \notin \Omega} I(uv) + 2\sqrt{1 - \frac{2}{3+2}} + 2\sqrt{1 - \frac{2}{3+2}} + \sqrt{1 - \frac{2}{3+d_T(u_4)}}.$$

Thus,

$$\begin{aligned} ABSC(T) - ABSC(T^*) &> 3\sqrt{1 - \frac{2}{4+2}} - 2\sqrt{1 - \frac{2}{3+2}} + \sqrt{1 - \frac{2}{2+1}} \\ &\quad - 2\sqrt{1 - \frac{2}{2+2}} > 0. \end{aligned}$$

Case 3. $t \geq 5$.

For $t \geq 5$, we consider further two cases, $q_i \neq u_{t-1}^{l_{t-1}}$ and $q_i = u_{t-1}^{l_{t-1}}$. First we consider $q_i \neq u_{t-1}^{l_{t-1}}$. Let $\Omega = \{uu_i^0, u_i^{l_i}u_i^{l_i-1} \mid 1 \leq i \leq t-1\} \cup \{q_iq, uu_t\}$. Let $T^* = T - \{uu_1^0, uu_2^0, l \dots, uu_{t-1}^0\} + \{u_1^0q_i, u_2^0u_1^{l_1}, u_3^0u_2^{l_2}, l \dots, u_{t-1}^0u_{t-2}^{l_{t-2}}\}$. Then we have $|V(T^*)| = n$ and $\Delta(T^*) = \Delta$. Thus we have

$$\begin{aligned} ABSC(T) &= \sum_{uv \notin \Omega} I(uv) + \sum_{uv \in \Omega} I(uv) \\ &= \sum_{uv \notin \Omega} I(uv) + (t-1)\sqrt{1 - \frac{2}{2+1}} + \sqrt{1 - \frac{2}{2+1}} \\ &\quad + (t-1)\sqrt{1 - \frac{2}{t+2}} + \sqrt{1 - \frac{2}{t+d_T(u_t)}} \end{aligned}$$

and

$$\begin{aligned} ABSC(T^*) &= \sum_{uv \notin \Omega} I(uv) + (t-1)\sqrt{1 - \frac{2}{2+2}} + \sqrt{1 - \frac{2}{2+1}} \\ &\quad + (t-1)\sqrt{1 - \frac{2}{2+2}} + \sqrt{1 - \frac{2}{1+d_T(u_t)}}. \end{aligned}$$

Thus,

$$ABSC(T) - ABSC(T^*) > (t-1) \left[\sqrt{\frac{1}{3}} + \sqrt{1 - \frac{2}{t+2}} - \sqrt{2} \right] > 0, \text{ for } t \geq 5.$$

Now suppose that $q_i = u_{t-1}^{l_{t-1}}$. Let $T^* = T - \{uu_1^0, uu_2^0, l \dots, uu_{t-2}^0\} +$

$\{u_1^0 q_i, u_1^{t_1} u_2^0, u_2^{l_2} u_3^0, l \dots, u_{t-3}^{l_{t-3}} u_{t-2}^0\}$. Then $|V(T^*)| = n$ and $\Delta(T^*) = \Delta$. Let $\Omega = \left\{uu_i^0, u_i^{l_i} u_i^{l_i-1} \mid 1 \leq i \leq t-1\right\} \cup \{uu_t\}$. Then we have

$$\begin{aligned} ABSC(T) &= \sum_{uv \notin \Omega} I(uv) + \sum_{uv \in \Omega} I(uv) \\ &= \sum_{uv \notin \Omega} I(uv) + (t-1) \sqrt{1 - \frac{2}{1+2}} + (t-1) \sqrt{1 - \frac{2}{t+2}} \\ &\quad + \sqrt{1 - \frac{2}{t+d_T(u_t)}} \end{aligned}$$

and

$$\begin{aligned} ABSC(T^*) &= \sum_{uv \notin \Omega} I(uv) + (t-2) \sqrt{1 - \frac{2}{2+2}} + \sqrt{1 - \frac{2}{1+2}} \\ &\quad + (t-1) \sqrt{1 - \frac{2}{2+2}} + \sqrt{1 - \frac{2}{2+d_T(u_t)}}. \end{aligned}$$

Thus,

$$\begin{aligned} ABSC(T) - ABSC(T^*) &> (t-2) \left(\sqrt{\frac{1}{3}} - \sqrt{\frac{1}{2}} \right) \\ &\quad + (t-1) \left(\sqrt{1 - \frac{2}{t+2}} - \sqrt{\frac{1}{2}} \right) > 0, \text{ for } t \geq 5. \end{aligned}$$

This completes the proof. ■

A *spider* is a tree with only one vertex whose degree is greater than two and that vertex is called the central vertex of the spider. A leg in a spider is a path from the vertex with maximum degree to one pendent vertex.

Lemma 9. *Let T be a spider with n vertices and $k \geq 3$ legs. If there is a leg of length larger than two and a leg of length one. Then there exists a spider T^* with k legs and n vertices such that $ABSC(T) > ABSC(T^*)$.*

Proof. Let T be a spider and r be the central vertex and root of T . Also, we let $N_T(r) = \{r_1, r_2, \dots, r_k\}$. Without loosing the generality, we can

suppose that $r_k y_1 y_2 \dots y_l$ is the most longest leg of spider T . Consider a set $\Omega = \{r_1 r, y_l y_{l-1}, y_{l-2} y_{l-1}\}$. Let $T^* = T - y_l y_{l-1} + r_1 y_l$. Then we have

$$\begin{aligned} ABSC(T) &= \sum_{uv \notin \Omega} I(uv) + \sum_{uv \in \Omega} I(uv) \\ &= \sum_{uv \notin \Omega} I(uv) + \sqrt{1 - \frac{2}{k+1}} + \sqrt{1 - \frac{2}{1+2}} + \sqrt{1 - \frac{2}{2+2}} \end{aligned}$$

and

$$ABSC(T^*) = \sum_{uv \notin \Omega} I(uv) + \sqrt{1 - \frac{2}{k+2}} + \sqrt{1 - \frac{2}{1+2}} + \sqrt{1 - \frac{2}{1+2}}.$$

Thus,

$$\begin{aligned} ABSC(T) - ABSC(T^*) &= \sqrt{1 - \frac{2}{k+1}} - \sqrt{1 - \frac{2}{k+2}} + \sqrt{1 - \frac{2}{2+2}} \\ &\quad - \sqrt{1 - \frac{2}{1+2}} > 0, \text{ for } k \geq 3. \end{aligned}$$

This completes the proof. ■

Now we can prove Theorem 4 by using the above lemmas.

Proof of Theorem 4. Let $T^* \in \mathcal{T}_{n,\Delta}$ ($n \geq 5$) and $ABSC(T^*) = \min \{ABSC(T) \mid T \in \mathcal{T}_{n,\Delta}, n \geq 5\}$. Let r be the root of T^* with $\Delta T^* = \Delta$. If $\Delta = 2$, then $T \cong P_n$. By Lemma 1, the conclusion holds. We may suppose $\Delta \geq 3$. By our choice of T^* as minimum of $ABSC(T)$, we conclude from Lemmas 6, 7 and 8 that T^* is a spider having central vertex r . Further we have two cases now:

Case 1. All legs of T^* have length at least two.

It is obvious $\Delta \leq \frac{n-1}{2}$, thus

$$\begin{aligned} ABSC(T^*) &= \Delta \sqrt{1 - \frac{2}{\Delta+2}} + \Delta \sqrt{1 - \frac{2}{1+2}} \\ &\quad + (n - 2\Delta - 1) \sqrt{1 - \frac{2}{2+2}} \end{aligned}$$

$$= \Delta \left(\sqrt{\frac{\Delta}{\Delta+2}} + \sqrt{\frac{1}{3}} \right) + \frac{\sqrt{2}}{2} (n - 2\Delta - 1).$$

Case 2. All legs of T^* have length at most 2.

From Case 1, we can suppose that T^* has at least one leg of length 1. If T^* is a star graph then the result will be obvious, so suppose that T^* is not a star graph. Then the number of leaves in $N_{T^*}(r)$ are $2\Delta + 1 - n$ and we have:

$$\begin{aligned} ABSC(T) &= (2\Delta - n + 1) \sqrt{1 - \frac{2}{\Delta + 1}} + (n - \Delta - 1) \sqrt{1 - \frac{2}{\Delta + 2}} \\ &\quad + (n - \Delta - 1) \sqrt{1 - \frac{2}{1 + 2}} \\ &= (n - \Delta - 1) \left(\sqrt{\frac{\Delta}{\Delta + 1}} + \sqrt{\frac{1}{3}} \right) + (2\Delta - n + 1) \sqrt{\frac{\Delta - 1}{\Delta + 1}}, \end{aligned}$$

which completes our arguments. ■

3 Upper bounds for the *ABSC* index of graphs

In this section, we will consider some upper bounds for the atom-bond sum-connectivity index of graphs.

Theorem 5. *Let G be a connected graph having n vertices, m edges, maximum degree Δ , minimum degree δ , and clique number α . Then*

$$ABSC(G) \leq \frac{n^2(\alpha - 1)}{2\alpha} \sqrt{\frac{\Delta - 1}{\delta}}, \quad (11)$$

the equality holds if and only if G is a complete α -partite graph in which all classes are of equal cardinality.

Proof. We know that

$$ABSC(G) = \sum_{uv \in E(G)} \sqrt{1 - \frac{1}{d_u + d_v}} \leq m \sqrt{\frac{\Delta - 1}{\delta}},$$

since G has a clique number α , so G is $K_{\alpha+1}$ -free graph. By Lemma 4, we get

$$m \leq \frac{n^2(\alpha - 1)}{2\alpha},$$

so from the above arguments we get our required result. Suppose that the equality holds in (11). We can conclude that G is a complete α -partite graph in which all the classes are of equal cardinality.

Conversely, if G is a complete α -partite graph in which all the classes are of equal cardinality, then

$$ABSC(G) = \frac{n^2(\alpha - 1)}{2\alpha} \sqrt{\frac{\Delta - 1}{\delta}},$$

which completes our arguments. ■

Lemma 10. ([2]) *Let G be a graph with m edges. Then*

$$ABSC(G) \leq \sqrt{m(m - H(G))}, \quad (12)$$

the equality holds if and only if either $m = 0$ or there is a fixed number k' such that $d_u + d_v = k'$ for every edge $uv \in E(G)$.

Theorem 6. *Let G be a simple graph with m edges and chromatic number $\chi(G)$. Then*

$$ABSC(G) \leq m \sqrt{1 - \frac{\chi(G)}{2m}},$$

the equality holds if and only if G is a complete graph possibly with the some additional isolated vertices.

Proof. By Lemmas 5 and 10, we have

$$\begin{aligned} \frac{\chi(G)}{2} &\leq \frac{m^2 - (ABSC(G))^2}{m}, \\ (ABSC(G))^2 &\leq m^2 - \frac{m\chi(G)}{2}, \\ ABSC(G) &\leq m \sqrt{1 - \frac{\chi(G)}{2m}}. \end{aligned}$$

This completes the proof. ■

4 Conclusions

In this paper, we first presented some lower bounds for the *ABSC* index of graphs especially for the trees with given maximum degree. Then we gave some upper bounds for the *ABSC* index of graphs. We found sharp bounds in terms of different graph parameters such as the first Zagreb index, the harmonic index, the sum-connectivity index, the minimum and maximum degrees, the clique number, and the chromatic number. The problem of finding the maximum *ABSC* index of trees with given maximum degree and characterizing the extremal trees remain to be resolved in the future.

Acknowledgment: he first author is grateful to Professor Shenggui Zhang for his constant support and guidance. Research was partially supported by the the Natural Science Foundation of Hubei Province (No. 2025AFD-006), the Foundation of Hubei Provincial Department of Education (No. Q20232505) and the Hubei Province University's outstanding young and middle-aged scientific and technological innovation team project (Grant No. T2023020).

References

- [1] A. Ali, K. C. Das, D. Dimitrov, B. Furtula, Atom-bond connectivity index of graphs: a review over extremal results and bounds, *Discr. Math. Lett.* **5** (2021) 68–93.
- [2] A. Ali, B. Furtula, I. Redžepović, I. Gutman, Atom-bond sum-connectivity index, *J. Math. Chem.* **60** (2022) 2081–2093.
- [3] A. Ali, I. Gutman, I. Redžepović, Atom-bond sum-connectivity index of unicyclic graphs and some applications, *El. J. Math.* **5** (2023) 1–7.
- [4] A. Ali, I. Z. Milovanović, E. Milovanović, M. Matejić, Sharp inequalities for the atom-bond (sum) connectivity index, *J. Math. Ineq.* **17** (2023) 1411–1426.
- [5] A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, New York, 2008.
- [6] K. C. Das, I. Gutman, B. Furtula, On atom-bond connectivity index, *Chem. Phys. Lett.* **511** (2011) 452–454.

-
- [7] H. Deng, S. Balachandran, S. K. Ayyaswamy, Y. B. Venkatakrishnan, On the harmonic index and the chromatic number of a graph, *Discr. Appl. Math.* **161** (2013) 2740–2744.
- [8] M. V. Diudea, I. Gutman, L. Jantschi, *Molecular Topology*, Nova, Huntington, 2001.
- [9] Y. Gao, Y. Shao, The smallest ABC index of trees with n pendent vertices, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 141–158.
- [10] Y. Ge, Z. Lin, J. Wang, Atom-bond sum-connectivity index of line graphs, *Discr. Math. Lett.* **12** (2023) 196–200.
- [11] K. J. Gowtham, I. Gutman, On the difference between atom-bond sum-connectivity and sum-connectivity indices, *Bull. Cl. Sci. Math. Nat. Sci. Math.* **47** (2022) 55–65.
- [12] E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.* **319** (2000) 713–718.
- [13] E. Estrada, Atom-bond connectivity and the energetic of branched alkanes, *Chem. Phys. Lett.* **463** (2008) 422–425.
- [14] E. Estrada, The ABC matrix, *J. Math. Chem.* **55** (2017) 1021–1033.
- [15] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian J. Chem.* **37A** (1998) 849–855.
- [16] S. Fajtlowicz, On conjectures of Graffiti II, *Congr. Num.* **60** (1987) 187–197.
- [17] B. Furtula, I. Gutman, M. Ivanović, D. Vukičević, Computer search for trees with minimal ABC index, *Appl. Math. Comput.* **219** (2012) 767–772.
- [18] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
- [19] S. A. Hosseini, B. Mohar, M. B. Ahmadi, The evolution of the structure of ABC-minimal trees, *J. Comb. Theory Ser. B* **152** (2022) 415–452.
- [20] H. Hua, K. C. Das, H. Wang, On atom-bond connectivity index of graphs, *J. Math. Anal. Appl.* **479** (2019) 1099–1114.

-
- [21] Y. Hu, F. Wang, On the maximum atom-bond sum-connectivity index of trees, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 709–723.
- [22] W. Lin, J. Chen, Z. Wu, D. Dimitrov, L. Huang, Computer search for large trees with minimal ABC index, *Appl. Math. Comput.* **338** (2018) 221–230.
- [23] F. Li, Q. Ye, H. Lu, The greatest values for atom-bond sum-connectivity index of graphs with given parameters, *Discr. Appl. Math.* **344** (2024) 188–196.
- [24] D. S. Mitrinović, P.M. Vasić, *Analytic Inequalities*, Springer-Verlag, Berlin, 1970.
- [25] P. Nithya, S. Elumalai, S. Balachandran, S. Mondal, Smallest ABS index of unicyclic graphs with given girth, *J. Appl. Math. Comput.* **69** (2023) 3675–3692.
- [26] P. Nithya, S. Elumalai, S. Balachandran, Minimum atom-bond sum-connectivity index of unicyclic graphs with maximum degree, *Discr. Math. Lett.* **13** (2024) 82–88.
- [27] S. Noureen, A. Ali, Maximum atom-bond sum-connectivity index of n -order trees with fixed number of leaves, *Discr. Math. Lett.* **12** (2023) 26–28.
- [28] M. Randić, Characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.
- [29] P. Turán, An extremal problem in graph theory, *KöMaL* **48** (1941) 436–452.
- [30] Y. Zhang, H. Wang, G. Su, K. C. Das, Extremal problems on the atom-bond sum-connectivity indices of trees with given matching number or domination number, *Discr. Appl. Math.* **345** (2024) 190–206.
- [31] B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270.